Quantum process tomography: the role of initial correlations

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We address the problem of quantum process tomography with the preparators producing states correlated with the environmental degrees of freedom that play role in the system-environment interactions. We discuss the physical situations, in which the dynamics is described by nonlinear, or noncompletely positive transformations. In particular, we show that arbitrary mapping $\varrho_{\rm in}\to\varrho_{\rm out}$ can be realized by using appropriate set of preparators and applying the unitary operation SWAP. The experimental "realization" of perfect NOT operation is presented. We address the problem of the verification of the compatibility of the preparator devices with the estimating process. The evolution map describing the dynamics in arbitrary time interval is known not to be completely positive, but still linear. The tomography and general properties of these maps are discussed.

I. MOTIVATION

The postulates of quantum theory require that the dynamics of isolated quantum systems is driven by Schrödinger equation [1, 2], i.e. for each time interval the evolution is described by a unitary transformation. However, for open quantum systems the situation is different [3, 4] and under certain assumptions the evolution is described as an one-parametric sequence of completely positive tracepreserving linear maps (quantum channels) $\mathcal{E}_t$. These mappings describe the state dynamics for arbitrary time interval $(0,t)$, however for general time intervals (t_1,t_2) the state transformations $\mathcal{E}_{t_1,t_2}:\varrho_{t_1}\to\varrho_{t_2}$ do not necessarily possess the above property of complete positivity. The aim of this paper is to analyze the cases, in which the description of quantum dynamics is not completely positive, or even not linear. One of the discussed problems will be the question of properties of the evolution map $\mathcal{E}_{t_1,t_2}$ for intermediate time intervals for general dynamics of open system governed by sequence $\mathcal{E}_t$. An important exception is if the sequence $\mathcal{E}_t$ fulfills the semigroup property, i.e. $\mathcal{E}_{t+s}=\mathcal{E}_t\mathcal{E}_s$ for all $t,s\geq 0$. In this case for each intermediate time interval the dynamics is linear and completely positive.

The lack of complete positivity and linearity for state transformations is usually interpreted as an unphysical property, i.e. these operations cannot be physically realized. But still an optimal physical approximation of several physically impossible processes is of great importance. Typical examples are quantum NOT operation [5], quantum copy operation [6, 7], etc. These processes violate the rules of quantum dynamics. However, we will see under which circumstances and in which sense even such unphysical transformations can be observed in our labs.

Quantum process tomography is a particular goal of quantum experiments. Several strategies how to gather valuable experimental data for this task and methods how to correctly proceed such data are known [8–14]. The failure of the direct (inverse) estimation methods that could result in an unphysical map [9, 13], is usually corrected by usage of more sophisticated statistical tools such as maximum likelihood [10, 11], or Bayesian statistics [12]. These methods are "forced" to lead to a correct quantum channel. We used to say that the failure of the direct estimation schemes follows from the finiteness of the measured statistical sample, i.e. the observed frequencies do not correspond to theoretically allowed probabilities and consequently, they do not correspond to some completely positive tracepreserving linear map. Here we shall address the question, under which circumstances such "unphysicality" can be due to imperfect (potentially correlated) preparators.

II. NONIDEAL PREPARATIONS

The usual picture of open quantum system dynamics is based on three assumptions: i) the physical object under consideration is a part of some larger system that is isolated, i.e. its evolution is unitary, ii) initial state of the object and the environment is factorized, and iii) the state of the environment is independent of the state of the system. Under such conditions the resulting dynamics is completely positive and linear. The question is whether the unphysical maps obtained as a result of direct estimation can be interpreted in this picture provided that we relax the last two conditions, i.e. the initial state is potentially correlated, or the state of the environment depends on the system state, or both. This question, namely how the initial correlations affect the dynamics of open system, has been already studied by several authors [15–20]. Authors in [17, 19, 20] analyze this problem and propose the mathematical tools how to mathematically describe such extended evolution maps.

A general state of bipartite system can be written in the following form

$$\varrho_{AB}=\varrho_A\otimes\varrho_B+\sum_{jk}\Gamma_{jk}\Lambda_j^A\otimes\Lambda_k^B \qquad (2.1)$$

where $\Lambda_0^X=\frac{1}{\dim\mathcal{H}_X}I$, ${\rm Tr}\Lambda_j^X\Lambda_k^X=\delta_{jk}$ with $X=A,B$, $j=0,1,\dots,\dim\mathcal{H}_A-1$ and $k=0,1,\dots,\dim\mathcal{H}_B-1$. Co-

efficients $\Gamma_{jk} = \langle \Lambda_j^A \otimes \Lambda_k^B \rangle_{\varrho_{AB}} - \langle \Lambda_j^A \rangle_{\varrho_A} \langle \Lambda_k^B \rangle_{\varrho_B}$ form the so-called correlation matrix. The evolution $\mathcal{E}$ of the subsystem A is a composition of the following three maps: 1) preparation map [21] $\mathcal{P} : \mathcal{S}_A \to \mathcal{S}_{AB}$ ($\mathcal{S}_X$ stands for the set of quantum states of the system X) satisfying the property $\mathrm{Tr}_B \mathcal{P}[\varrho_A] = \varrho_A$, 2) isolated dynamics $\mathcal{U} : \mathcal{S}_{AB} \to \mathcal{S}_{AB}$, i.e. $\varrho'_{AB} = \mathcal{U}[\varrho_{AB}] = U \varrho_{AB} U^\dagger$, and 3) partial trace $\mathcal{T}_B : \mathcal{S}_{AB} \to \mathcal{S}_A$. The last two mappings are linear and completely positive. Moreover, both of these two features are preserved under the composition of mappings. That is, the only source of "nonphysicality" is the preparation map $\mathcal{P}$. One can show [15] that the linearity of the resulting dynamical map $\mathcal{E} = \mathcal{T}_B \circ \mathcal{U} \circ \mathcal{P}$ requires $\mathcal{P}$ be of the form $\mathcal{P}[\varrho_A] = \varrho_A \otimes \xi_B$ with ξ_B arbitrary, but fixed. In such case the linearity and complete positivity of $\mathcal{E}$ holds.

In [20] authors studied different types of preparation maps and define the notion of an accessible map. The transformation is called accessible if it can be written as a composition of the preparation, unitary transformation and partial trace [22]. If one allows arbitrary initial correlations, then the transformation is composed of two terms [16]

$$\varrho'_A = \sum_{\mu\nu} A_{\mu\nu} \varrho A^\dagger_{\mu\nu} + \sum_{jk} \Gamma_{jk} \sum_{\mu} \langle \mu | \Lambda_j^A \otimes \Lambda_k^B | \mu \rangle \, . \quad (2.2)$$

where the operators $A_{\mu\nu} = \langle \mu | \sqrt{p_\nu} U | \nu \rangle$ depends on ϱ_B, because $|\mu\rangle$ are eigenvectors of the operator ϱ_B. That is, even if we put $\Gamma = 0$, the transformation $\varrho_A \to \varrho'_A$ is still not necessarily described by some proper quantum channel, because the choice of ϱ_B specifying the preparation map $\mathcal{P}$ can depend on ϱ_A. Consider an arbitrary state transformation $\varrho_{in} \to \varrho_{out}$. Let us define a preparation in the following way $\mathcal{P}[\varrho_{in}] = \varrho_{in} \otimes \varrho_{out}$. Next apply the SWAP operation (this is a unitary transformation) to obtain $U_{\mathrm{SWAP}}(\varrho_{in} \otimes \varrho_{out}) U^\dagger_{\mathrm{SWAP}} = \varrho_{out} \otimes \varrho_{in}$. After performing the partial trace we obtain the required state transformation $\varrho_{in} \to \varrho_{out}$. Moreover, we did not use any correlation (quantum, or classical) in our preparation at all. Of course, this construction is a bit artificial, but nevertheless it shows that arbitrary state transformation $\varrho_{in} \to \varrho_{out}$ is in principle accessible, i.e. can be written as $\mathcal{T}_B \circ \mathcal{U} \circ \mathcal{P}$. In order to avoid such "artificial" realizations of any map we need to pose some well-motivated physical conditions. In the Ref.[17, 19, 20] the authors restrict themselves to linear preparation maps. In what follows we will analyze two experimental situations in which a preparation map is naturally defined and the extended dynamics can be studied.

Before we get further let us mention one very important implication of the fact that arbitrary channel is accessible. In a sense this statement is very positive, because whenever we find out in our experiments some strong evidence that the dynamics is not linear, or not completely positive, we cannot automatically conclude that the quantum theory is not correct. The observed "unphysicality" can be still interpreted as the problem of devices called preparators that produce states correlated to degrees of freedom relevant for the subsequent system evolution. Without considering the dynamics the potential correlations are not interesting and from kinematic point of view they are irrelevant. However, these dynamical aspects can be used to differentiate between otherwise kinematically equivalent preparators. From this point of view the "nonphysicality" means that the preparators are not independent of the environmental degrees of freedom that do take a role in the dynamics.

As an example consider now the realization of the perfect NOT operation realized on pure states $|\psi\rangle \to |\psi_\perp\rangle$. Let us assume that the preparation of the spin-$\frac{1}{2}$ pure state is performed by a postselection after Stern-Gerlach measurement. In this way we can prepare any pure quantum state and mixtures can be obtained by mixing the pure state preparations. Kinematically this is completely correct preparation procedure of arbitrary qubit state. Imagine a situation that the spin is entangled with another spin such that together they are described by the singlet, i.e. $|\Psi\rangle = \frac{1}{\sqrt{2}}(|\psi\rangle|\psi_\perp\rangle - |\psi_\perp\rangle|\psi\rangle)$. Reading the outcome tells us perfectly which state $|\psi\rangle$ we prepared, but the measurement affects also the state of the second spin, which is described by the state $|\psi_\perp\rangle$. If the unknown device internally just swaps these two spins, than we find out that the device performs the transformation $|\psi\rangle \to |\psi_\perp\rangle$, i.e. the perfect NOT operation. Experimenter using such preparations is not aware of the initial correlations and therefore he would conclude that the unknown device performs perfect quantum NOT operation. This conclusion is not wrong and indeed experimenter can prove that this device performs NOT operation, but only for specific preparation procedures. If he would use different state preparators (i.e. kinematically equivalent to the previous ones), he will very soon find some contradiction.

III. PROCESS TOMOGRAPHY

The "nonphysicality" is not an exception in process tomography using the direct estimation schemes [24]. In such schemes we usually measure a collection of assignments $\varrho_j \to \varrho'_j$ for linearly independent states $\{\varrho_j\}$. Using the linearity of quantum channels these assignments provide us with sufficient information to complete the reconstruction task. In other words: each state ϱ can be written as a linear combination of states ϱ_j, i.e. $\varrho = \sum_j a_j \varrho_j$ (a_j are arbitrary). Therefore the transformation of ϱ is determined by the set of measured assignments. However, quite often the resulting map is not completely positive. Even in cases when all ϱ_j, ϱ'_j are proper quantum states. A reason could be really only the usage of finite data sample, i.e. the statistics is really small to conclude something about actual probabilities, mean values, and states. This line of arguments leads us to the usage of sophisticated statistical techniques (maximum likelihood, Bayesian approach, etc.). These statistical methods are modified for quantum tomogra-

phy purposes in a way that they are essentially forced to guarantee a physically valid result (a completely positive map in quantum process tomography) even in situations when the direct inverse schemes fail. However, as we have just explained, this lack of complete positivity can be due to presence of correlations in our preparators as well. If this is the case it is really not easy to say which of the preparators are not perfect, i.e. which of them represent the source of nonphysicality. It could happen that only one of them is imperfect, or all of them are imperfect.

Without any insight into the physics behind the preparation process, the measured data do not contain any information about the origins and form of the preparation map. As we have seen there is always a trivial example using the SWAP operation that can be used to interpret arbitrary result. It is important to say here, that even if the "linearization" of assignments gives a correct quantum channel, it does not mean that our preparators are perfect. We should have in mind that the linearity is not tested, but only used as the theoretical tool to accomplish the process estimation. In order to be sure about linearity one really needs to test the action of the channel on preparators of any quantum state. In this sense the specification of the channel is always only a hypothesis and for specific (imperfect) preparators we can find the channel to be "unphysical". Important point is that the usual notion of quantum channel has a good meaning only for properly prepared input states, i.e. for compatible preparators.

We said that using only the measured data we have only very partial information about the real physics of the process. There are many possible unitary representations of the observed assignments. One of the option is to say that a collection of used preparators was not perfect and conclude that the process estimation is not possible. Another approach is to apply some techniques of incomplete process tomography [27] to estimate the unitary map acting on the system with Hilbert space $\mathcal{H}\otimes\mathcal{H}_{\rm env}$, where $\mathcal{H}_{\rm env}$ is arbitrary. However this is indeed a difficult task, because we need to deal with data that do not contain complete information about the inputs as well as about the outputs of the channel, i.e. the assignments are not completely known. The method that can be used in such situations is called principle of maximum entropy [28]. However, these issues are beyond the scope of this paper.

IV. COMPATIBILITY OF PREPARATOR AND TESTED PROCESS

To be sure that the channel estimation gives a physical result one needs to use the collection of "good" preparators producing linearly independent test states. "Good" in a sense that whatever degrees of freedom enters the preparation process, these are irrelevant for the channel realization. We will say that such preparators are compatible with the channel realization. Let us note that the condition of producing a factorized state is not sufficient, i.e. even pure state preparators are not automatically free of imperfections. This follows from the example with SWAP operation, where no correlations in preparator process are used at all, but any transformation can be realized. We see that important question is: how to test the quality of the preparator, or better to say, how to test the compatibility of the preparator and the quantum process?

The motivation for the scheme we are going to use comes from the preparation process used in real experiments [25, 26, 29, 30]. In some cases the preparation of different states is done by exploiting quantum processing, i.e. transforming the known state by a known transformation to obtain a new state. In particular, let us assume we have a preparator that produces system in a state ϱ. Applying unitary rotations U_j we are able to prepare states $\varrho_j = U_j\varrho U_j^\dagger$ that can be used to test the properties of an unknown quantum channel. Our aim is to test the compatibility of the original preparator and some unknown device (black box). Except the case of $\varrho=\frac{1}{d}I$ the unitary processing produce sufficiently many linearly independent states to perform the complete process tomography. This procedure, of course, requires perfect realization and control of unitary transformations U_j. Moreover, these unitaries must be already "compatible" with the preparator. In some sense we are cheating a bit here, because we are going to test the compatibility of the preparator with a given device and we already assume we have devices (performing unitaries) compatible with the preparator. However, as we said this is quite usual procedure how to prepare different states in many experiments. Therefore, let us assume that we indeed have such compatible devices. Then the described setting can be used to test the quality of the single preparator with respect to the realization of the unknown channel $\mathcal{E}$. Important point is that these "preparing operations" are independent of the original preparator, i.e. they do not introduce the "unphysicality" and the only source of "unphysicality" is the preparator of ϱ. Let us note that there is no need for preparing operations to be unitary, but in general, they must be linear and completely positive in order not to introduce extra sources of "unphysicality".

In what follows we will study the properties of the preparation map given the described model of the experiment consisting of a preparator, an unknown black box $\mathcal{E}$ and a set of preparing operations $\{\Phi\}$ (not necessarily unitary ones). Consider that the original preparator (the one we want to test with respect to the channel action) produces states $\omega = \varrho\otimes\varrho_B+\Gamma$, where $\Gamma=\sum_{jk}\Gamma_{jk}\Lambda_j\otimes\Lambda_k$ stands for the correlations. After fixing the set of preparing operations $\{\Phi\}$ the preparation $\mathcal{P}$ is, in general, defined as follows

$$\mathcal{P}:\varrho_\Phi\mapsto\omega_\Phi=\Phi\otimes\mathcal{I}[\omega]=\varrho_\Phi\otimes\varrho_B+\Gamma' \qquad (4.1)$$

with $\Gamma'=\Phi\otimes\mathcal{I}[\Gamma]=\sum_{jk}\Gamma'_{jk}\Lambda_j\otimes\Lambda_k$ ($\Gamma'_{jk}=\sum_l\Phi_{jl}\Gamma_{lk}$, $\Phi_{jl}={\rm Tr}(\Lambda_j\Phi[\Lambda_k])$) and $\varrho_\Phi=\Phi[\varrho]$. The possible preparation mappings $\mathcal{P}$ are represented by subsets of com-

pletely positive tracepreserving linear maps Φ that transform the given state ϱ into arbitrary state in the domain of $\mathcal{P}$. The simple example with the SWAP gate is excluded/trivial in this case, because it generates only contractions into the fixed state ϱ_B. Moreover, the correlations induced in the preparation process are in some sense fixed by the state ω, i.e. by the original state preparator that we are testing (together with the channel reconstruction).

The unitary evolution $U=\sum_{\mu,\nu} A_{\mu\nu}\otimes|\mu\rangle\langle\nu|$ induces the state transformation

$$\varrho_\Phi \to \varrho'_\Phi = \sum_{\mu,\nu} \lambda_\nu A_{\mu\nu}\varrho_\Phi A^\dagger_{\mu\nu} + \sum_{j,k,\mu,\nu,\nu'} \Gamma'_{jk}[\Lambda_k]_{\nu\nu'} A_{\mu\nu}\Lambda_j A^\dagger_{\mu\nu'} \quad (4.2)$$

where we used that $\varrho_B = \sum_\nu \lambda_\nu|\nu\rangle\langle\nu|$, i.e. $\{|\nu\rangle\}$ are eigenvectors of ϱ_B. Since ϱ_B is fixed for any operation Φ we see that the first term is independent of Φ, i.e. it is independent of the preparation map $\mathcal{P}$. Consequently, the unknown transformation $\mathcal{E}$ describing the device can be written as the sum of linear completely positive map $\mathcal{F}$ ($\mathcal{F}[\varrho]=\sum_{\mu\nu} F_{\mu\nu}\varrho F^\dagger_{\mu\nu}$ with $F_{\mu\nu}=\sqrt{p_\nu}A_{\mu\nu}$) and some traceless operator [20] $\Xi_\varrho = \sum_{j,k,\mu,\nu,\nu'}\Gamma'_{jk}[\Lambda_k]_{\nu\nu'}A_{\mu\nu}\Lambda_j A^\dagger_{\mu\nu'}$, i.e. $\varrho\to\varrho'=\mathcal{E}[\varrho]=\mathcal{F}[\varrho]+\Xi_\varrho$. First part is irrelevant of the correlations, but the second part can be even nonlinear. The properties of Ξ_ϱ depends completely on the choice of the set of preparing operations Φ, i.e. choice of preparation mapping $\mathcal{P}$. In special cases it can be linear and not factorized, but then it cannot be defined on the whole state space. The linear case was analyzed in Ref.[20]), in which the sufficient conditions for its existence (in terms of properties of Ξ_ϱ) were formulated. The linearity of $\mathcal{P}$ corresponds to a specific choice of the set of preparing operations $\{\Phi\}$ for a given ω, but the specification of particular conditions remain to be an open problem.

Another open question is the characterization of all transformations (not only with linear preparation map $\mathcal{P}$) that can be understood within this model. This is indeed a very interesting, but also very difficult problem and we are not going to discuss this here. Our aim is to describe the idea how to test the compatibility of the original preparator and the action of an unknown device. The compatibility means that either the initial correlations vanish ($\Gamma=0$), or the unitary transformation generating the process dynamics is from the set of transformations $U\in\{U_A\otimes U_B, U_A\otimes U_B U_{\rm SWAP}\}$. The pure state preparators are specific examples of preparators with vanishing initial correlations ($\Gamma=0$), and using the described procedure the pure state preparators are always compatible with an arbitrary quantum process.

For instance, consider the preparator of a single pure state described in the example of the perfect NOT realization. That is, consider initially the spin is maximally entangled with another spin and by measuring along the z direction we are preparing the states $|\uparrow\rangle$. Instead of using different measurement apparatuses to generate arbitrary pure states, let us perform single qubit rotations of the state $|\uparrow\rangle$ to create arbitrary pure state $|\psi\rangle$. As before, the device just swaps the two spins, i.e. arbitrary $|\psi\rangle$ is replaced by $|\downarrow\rangle$. Consequently, the transformation we obtain in the single point contraction of the Bloch sphere, i.e. linear and completely positive map $\mathcal{E}[\varrho]=|\downarrow\rangle\langle\downarrow|$. That is, the same black box can be described by different quantum processes depending on the properties of the preparation procedures.

To test the dynamical compatibility of an unknown preparation device we suggest to exploit calibrated devices performing some well known quantum operations. In fact, this is nothing new, because the same procedure is used in most of the experiments. Important point is that using such method the properties of the resulting preparation map $\mathcal{P}$ (and consequently $\mathcal{E}$) strongly depends on the properties of the original preparator. If one observes some "unphysicality" of $\mathcal{E}$ in such experimental setting then before applying "statistical corrections" one should verify the compatibility of the preparator. Performing the process tomography experiment the set of preparing operations should be chosen in a way that the generated set of states is sufficient for the process tomography, i.e. this set is finite. The goal of the verification is to find whether the correlation matrix Γ vanishes, or not. There are, in principle, two strategies that can be combined. We can use different preparing operations Φ_1,Φ_2 generating the same state $\varrho_{\Psi_1}=\varrho_{\Phi_2}$ and see whether the channel action generates the same state. Alternatively, we can use additional preparing operations to verify the linearity. In order to see, whether the unphysicality is due to imperfections in the preparation process, a characterization of all preparation maps $\mathcal{P}$ in the described settings is needed. This characterization is an open problem the solution of which is necessary if we want to be able to propose some universal verification and estimation strategies.

V. EVOLUTION MAP FOR ARBITRARY TIME INTERVAL

Let us assume that the time evolution of the system is described by a set of completely positive maps $\mathcal{E}_t$ induced by some underlying unitary dynamics U_t of the system and its environment. This corresponds to a situation in which initially (time $t=0$) the system and the environment are factorized, i.e. $\omega_0=\varrho\otimes\xi$. Only under such assumption the maps $\mathcal{E}_t$ can be completely positive for all t and we have $\mathcal{E}_t={\rm Tr}U_t\varrho\otimes\xi U_t^\dagger$. In this section we turn back to the original question posed at the beginning: what are the properties of the time evolution maps $\mathcal{E}_{t_1,t_2}$ ($t_2>t_1$) describing the dynamics during arbitrary time interval $[t_1,t_2]$?

A direct calculation gives us that

$$\mathcal{E}_{t_1,t_2}[\varrho]=\mathcal{E}_{t_2}\circ\mathcal{E}^{-1}_{t_1}[\varrho]\,. \quad (5.1)$$

These maps are linear, tracepreserving and hermiticity preserving, and thus defined on any operator (quantum

state), but except $\varrho \in \mathcal{S} = \mathcal{E}_{t_1}[\mathcal{S}(\mathcal{H})] \subset \mathcal{S}(\mathcal{H})$ they can transform quantum states into negative operators. Following the notation of Refs.[17–20] we define the positivity domain $\mathcal{D}_{\rm pos}(\mathcal{E})$ of a linear map $\mathcal{E}$ as a subspace of states on which $\mathcal{E}$ is positive, i.e. $\mathcal{D}_{\rm pos}(\mathcal{E}) = \{\varrho \in \mathcal{S}(\mathcal{H}) : \mathcal{E}[\varrho] \geq 0\}$. In fact, physically, only the action on such subset is important, because this is what we can really test in our experiments. Let us note that $\mathcal{E}_{t_1}^{-1}$ corresponds to the mathematical inverse operation (not physical) and does not necessarily always exist. This means that the question about the form of $\mathcal{E}_{t_1,t_2}$ does not make sense if t_1 is a point in which the maps $\mathcal{E}_{t_1}$ is not invertible.

The described model illustrates another physical situation, in which the evolution map extended to whole state space is not completely positive. But in this case it is still linear, what makes its description much simpler. Moreover, since the evolution maps $\mathcal{E}_{t_1,t_2}$ preserves the trace and hermiticity, they can be expressed as a difference of two completely positive maps [17, 23]

$$\mathcal{E}_{t_1,t_2}[\varrho] = \sum_{j=1}^{q} A_j \varrho A_j^\dagger - \sum_{j=q+1}^{d^2} A_j \varrho A_j^\dagger \,, \tag{5.2}$$

where the operators A_j can be chosen so that they form an orthogonal operator basis (${\rm Tr} A_j^\dagger A_k = 0$ for $j \neq k$) and d is the Hilbert space dimension of the system. The tracepreservation is reflected by the identity $\sum_{j=1}^{q} A_j^\dagger A_j - \sum_{j=q+1}^{d^2} A_j^\dagger A_j = I$.

The physics behind such form of noncomplete positivity is simple and just reflects the fact that at time t_1 the system is correlated to relevant degrees of freedom that affects the forthcoming evolution. In each time instance t the global state of the system plus environment is described by some $\omega_t = U_t \omega_0 U_{-t}$. The preparation map in time t is determined by the choice of $\omega_0 = \varrho \otimes \xi$. In particular, $\mathcal{P}_t[\varrho_t] = \omega_t = U_t \omega_0 U_{-t} = U_t \mathcal{P}_0[\varrho_0] U_{-t} = U_t \mathcal{P}_0[\mathcal{E}^{-1}[\varrho_t]] U_{-t}$, i.e. $\mathcal{P}_t = \mathcal{U}_t \circ \mathcal{P}_0 \circ \mathcal{E}_t^{-1}$. That is, the evolution for time interval $(t, t+\delta t)$ can be written as follows

$$\mathcal{E}_{\delta t}[\varrho_t] = {\rm Tr}_B[U_{\delta t} \mathcal{P}_t[\varrho_t] U_{\delta t}^\dagger] = \mathcal{E}_{t+\delta t} \circ \mathcal{E}_t^{-1}[\varrho_t] \,. \tag{5.3}$$

Let us note that we can generalize the whole setting by allowing arbitrary preparation map $\mathcal{P}_0$, but we want to preserve the physical picture with the factorized preparation and therefore we will restrict ourselves to linear and factorized initial preparations only.

Before we get further let us note that the problem of quantum process tomography for linear noncompletely positive maps was discussed in dissertation of Anil Shaji [19]. To our knowledge this was the first attempt to understand the observed data in more general settings than just in the framework of completely positive maps. In particular, he analyzes the problem from the mathematical point of view. Since the maps of this form are linear, the reconstruction schemes based on complete data are the same independently whether the complete positivity constraint is applied, or not. The inverse estimation schemes use just the linearity of the quantum evolution and the observed data are collected so that the result is represented by some linear transformation uniquely. The only and crucial question is what type of linear transformation it is. According to usual model of open system dynamics we expect to obtain completely positive transformations in our experiments, but in reality this is not always the case [29, 30]. Of course, the origin of this phenomena is questionable, but correlations of preparation map within the discussed model provide one possible option. The estimation schemes and algorithms must be modified accordingly in cases, when indirect statistical methods (such as maximum likelihood, or Bayesian approach) are employed, or our information is incomplete. Those who are interested in the details of complete quantum process tomography for noncompletely positive, but linear maps we refer to [19]. In this paper we are proposing the corresponding physical situation specifying the conditions under which the linear noncompletely positive maps can be observed experimentally.

Our interest is not only to perform the process tomography experiment and reconstruction, but also to understand (at least partially) the physics behind. As we said the evolutions derived from the unitary dynamics U_t for a fixed time interval are linear, tracepreserving and also hermiticity preserving. Therefore, they are of the form as written in Eq.(5.2). We are interested in the inverse question, whether any such transformation $\mathcal{E}$ can be understand as subdynamics between two instants of time induced by some unitary dynamics. Or alternatively, under which circumstances the preparation mapping is linear on subset of quantum states and whether these situations can be always understand as part of the dynamics described by $\mathcal{E}_t$ derived from unitary dynamics U_t.

If we assume that the one-parametric family of unitaries U_t is arbitrary (i.e. the generating Hamiltonian is highly time dependent), then there are no constraints on the choice of the transformations $\mathcal{E}_t$ for different times. One can always define the generating unitary transformations U_t so that $\mathcal{T}_B \circ \mathcal{U}_t \circ \mathcal{P}_0 = \mathcal{E}_t$. Thus the question is, whether the following identity can be fulfilled $\mathcal{E}_{\delta t} = \mathcal{E}_{t+\delta t} \circ \mathcal{E}_t^{-1}$, where on the left hand side we have arbitrary linear transformation given by Eq.(5.2) and on the right hand side we have two arbitrary completely positive maps $\mathcal{E}_1, \mathcal{E}_2$. The inverse operation $\mathcal{E}_t^{-1}$ is linear, tracepreserving and hermiticity preserving as well, i.e. it serves as the potential source of noncomplete positivity. It is a well known fact that substraction of two completely positive maps realizes arbitrary noncompletely positive linear map (Eq.(5.2)), but here the question is whether a similar property holds for the "division" of two completely positive maps, i.e. for the transformation $\mathcal{E}_{t+\delta t} \circ \mathcal{E}_t^{-1}$.

Consider now the following example. The transposition $\mathcal{E}_{\rm trans}$ is probably the best known noncompletely positive linear map. Its action is defined as follows $\mathcal{E}_{\rm trans}[\varrho] = \varrho^T$ and for qubit it is closely related to perfect NOT operation. Let us assume that as the result of

the process tomography we obtain the NOT operation, $\mathcal{E}_{\rm NOT}[\varrho]=\frac{1}{2}(\sigma_x\varrho\sigma_x+\sigma_y\varrho\sigma_y+\sigma_z\varrho\sigma_z-\varrho)$. Could it happen within the discussed framework? Both these maps are positive, i.e. the positivity domain equals to the whole state space. In our settings the positivity domain always corresponds to an image of the whole state space under some completely positive map $\mathcal{E}_t$. However, only for unitary transformations the image of the state space equals to its original, i.e. if $\mathcal{E}_t$ is a linear completely positive map and $\mathcal{E}_t[\mathcal{S}(\mathcal{H})]=\mathcal{S}(\mathcal{H})$, then $\mathcal{E}_t$ is unitary. Therefore we have $\mathcal{E}_t=\mathcal{U}$. Because of the unitarity this process is invertible. Consequently, $\mathcal{E}_{t+\delta t}\circ\mathcal{E}_t^{-1}=\mathcal{E}_{t+\delta t}\circ\mathcal{U}^{-1}=\mathcal{E}_{\delta t}$ is necessarily a completely positive map. But this is in contradiction with the fact that our reconstruction gives us a noncompletely positive linear map $\mathcal{E}_{\rm NOT}$ (or $\mathcal{E}_{\rm trans}$). It means that the NOT operation $\mathcal{E}_{\rm NOT}$, or transposition $\mathcal{E}_{\rm trans}$ cannot be interpreted as an evolution map describing the time dynamics between two instants of time generated by a global unitary dynamics with initially factorized preparation map. In fact, the same conclusion holds for arbitrary positive (but not completely positive) linear map transforming pure states onto pure states, i.e. whenever the identity $\mathcal{E}[\mathcal{S}(\mathcal{H})]=\mathcal{S}(\mathcal{H})$ holds.

However, there is still an option how to "partially" perform the perfect NOT operation in the given framework of intermediate dynamics. The depolarizing single qubit channels form a one-parametric family $\mathcal{E}_{\{x\}}:\vec{r}\to x\vec{r}$, where $\vec{r}$ is the Bloch vector corresponding to a quantum state $\varrho=\frac{1}{2}(I+\vec{r}\cdot\vec{\sigma})$. For $x\in[-1/3,1]$ the transformations $\mathcal{E}_{\{x\}}$ are completely positive and $\mathcal{E}_{\rm NOT}=\mathcal{E}_{\{x=-1\}}$. For the inverse operations we have $\mathcal{E}_{\{x\}}^{-1}=\mathcal{E}_{\{1/x\}}$ and for the composition $\mathcal{E}_{\{y\}}\circ\mathcal{E}_{\{x\}}=\mathcal{E}_{\{x.y\}}$ for arbitrary real x,y. Using all these identities it simple to proof that $\mathcal{E}_{\rm NOT}=\mathcal{E}_{\{x\}}\circ\mathcal{E}_{\{-x\}}^{-1}=\mathcal{E}_{\{x.(-1/x)\}}=\mathcal{E}_{\{-1\}}$. This identity makes sense only for $-1/3\leq x\leq 1/3$, when both transformations are completely positive. Formally, the above calculation suggests that we are able to realize the perfect quantum NOT operation during the dynamics governed by one-parametric set of completely positive maps. But, the above decomposition possessed a physical meaning only for states from the subset $\mathcal{E}_{\{x\}}[\mathcal{S}(\mathcal{H})]$, i.e. for states with Bloch vectors smaller than $|x|$ ($|\vec{r}|\leq|x|$). The maximal set of states on which we are able to realize the perfect NOT operation (in the given model) is contained in the sphere with radius $x=1/3$. The conclusion is that the perfect NOT operation can be find out as a result of the process reconstruction. Moreover, it can be even understood as an intermediate dynamics, but it does not mean that the perfect NOT operation is indeed accomplished, because no intermediate dynamics can perform a perfect NOT operation for all set of states. Thus, process estimation of the quantum operation between two instants of time could result in perfect NOT operation. But the perfect NOT operation is performed only on restricted set of states.

Although the presented framework of open system dynamics enables us to explain quite naturally the experimental evidence of linear noncompletely positive maps, the answer to the inverse question is open, i.e. whether all hermiticity preserving, tracepreserving and linear transformations can be interpreted within the described model, if we relax its physical validity for the whole set of states. The characterisation of those noncompletely positive maps that can be realized within the discussed physical model is an open question that indeed requires deeper investigation.

VI. CONCLUSION

In this paper we have analyzed the dynamics of open quantum systems beyond the complete positivity restriction and related consequences for the process tomography. The correlations can be detected if the direct estimation procedure gives physically invalid result and simultaneously, all the experimental and statistical deviations can be excluded. The good news of our analysis is that any failure of the process estimation (i.e. "unphysical" result) cannot be interpreted as the failure of quantum theory unless one can exclude the presence of initial correlations and dynamically incompatible preparators. However, the particular realization using the SWAP operation is quite artificial. As an example, we have described two different experimental realizations of the perfect NOT gate, which is considered to be unphysical. The bad news is that although the initial correlations can be detected, the process tomography is very difficult and ambiguous, and the physical origin could be quite artificial. However, the usage of statistical tools is justified only if we can safely exclude all such (artificial) possibilities, i.e. we have some restrictions and models on the form of possible preparator maps.

We have discussed two very natural physical situations that can result in observation of initial correlations effect. First of them is motivated by current experiments, in which experimenters typically use single state preparator and other states are generated with the help of further processing, for instance by applying different unitary operations. In the second case the "unphysicality" is related to the fact that the evolution map describing the state dynamics during arbitrary time interval is in general not completely positive, but still it is linear. This situation is very closely related to experiments in process tomography, in which the state estimation of inputs is as necessary as the state estimation of the outputs, i.e. we indeed perform measurements in two time instants. And it could happen that already at the first time instant the system's and the channel's degrees of freedom are mutually (although weakly) correlated. Fortunately, from the practical point of view, in this case the process tomography schemes are not affected, only the data processing should be different if one uses some advanced statistical tools. We think that this framework provides a physically reasonable description for the existence of noncompletely positive linear maps. We have shown that in a strict sense not all linear noncompletely positive maps can be

indeed realized within such model. The question of the characterization of "accessible" maps within this model is interesting and very important, but unfortunately we do not know the answer yet.

We have argued that the problem of initial correlations is not a problem of quantum dynamics, but rather of quantum kinematics. In other words, the process tomography always describes a relation between the preparators and the channel. For different sets of preparators physically the same channel could be described by different dynamical maps. Only in very specific cases of preparators the channel is represented as a completely positive tracepreserving linear map. Fortunately, this is the case that usually holds in labs, or better to say, we are aiming to hold in our labs. We have described the method how to test the preparators using the calibrated quantum channels. Good preparator devices are crucial for the successful development of quantum information processing. The presented analysis is very far from being complete and a deeper investigation on the system-environment correlations effects on quantum dynamics and experiments is needed.

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